

Structural Information in Diffuse Diffraction Patterns

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The radiation diffraction pattern for amorphous materials requires special analysis for information on atomic groupings. Powdered crystalline material may also give diffuse patterns requiring this type of analysis. Absence of a sharp diffraction pattern does not necessarily indicate absence of the material. Examples are given for chrysotile and powdered chrysotile.

A diffraction pattern characteristic of a material is produced when that material interacts with a beam of radiation. This is true whether the material is ordered as a single crystal or amorphous as a glass. When asbestos minerals are subjected to mechanical and chemical treatment, their diffraction patterns often become quite diffuse. Considerable structural information may be obtained from such diffuse diffraction patterns. Silica glass will be used as an example.

Figure 1 illustrates the x-ray diffraction pattern of silica glass. As is characteristic for highly disordered systems, this diffraction pattern consists of a relatively few diffuse maxima. Interatomic distance information may be obtained directly from the diffraction pattern by means of Fourier analysis. For amorphous materials this distance information is in the form of a radial distribution function (RDF) that represents the distribution of interatomic distances within the sample (1).

However, subtle difficulties in the analysis can seriously interfere with the interpretation of the results. These difficulties arise in part from the limitations of the experimental data with respect to both the restricted range of scattering angle and accuracy. In addition, certain interferences can arise from the data and the subsequent Fourier analysis. Special

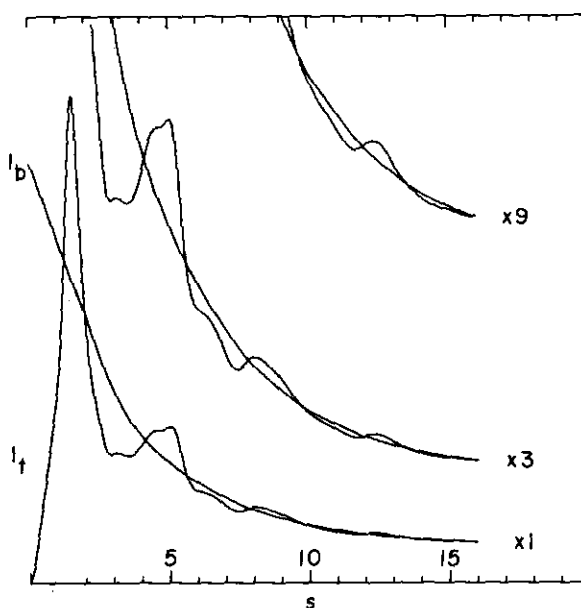


FIGURE 1. The x-ray diffraction pattern for silica glass. $S = 4\pi \sin\theta/\lambda$, where 2θ is the angle between the incident and diffracted beam and λ is the wavelength.

analytical procedures have to be employed to overcome these limitations (2).

Figure 2 illustrates the RDF obtained for silica glass. This RDF obtained from the diffuse diffraction pattern consists of features ranging from the very sharp maxima at 1.61 Å representing the bonded silicon-oxygen distances to the relatively broad features at about 18 Å

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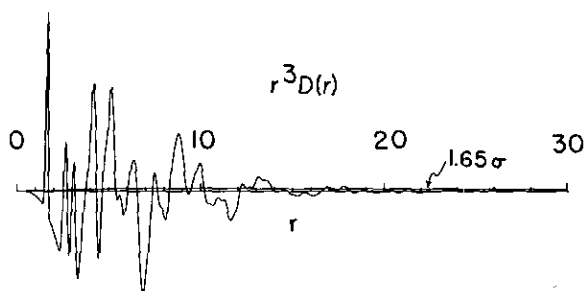


FIGURE 2. Radial distribution function for silica glass. The probability of atoms in the sample being separated by r Angstroms is obtained from $4\pi r^2 \rho(r)$, where $r^2 D(r) = 4\pi r^3 [\rho(r) - \rho_0]$ and ρ_0 is related to the bulk density.

Analysis of this RDF yielded information concerning the types of atomic groupings in the sample and the range over which they are ordered (3).

Figure 3 illustrates the powder diffraction patterns collected in our laboratory for chrysotile and chrysotile that has been ground under toluene for 1 hr. Upon further grinding, the diffraction pattern becomes progressively more diffuse. Preliminary microscopy indicates that the broadening is due not only to reduction in particle size, but also to disorder within the fibrils resulting in the loss of the periodicities that produced the sharp maxima. This type of disorder may occur with little change in particle size and local atomic order. It is therefore possible that micron size particles of chrysotile may give diffuse diffraction patterns due to slight misalignment of the atomic layers.

Caution should be exercised when attempting to identify from diffraction patterns an easily disordered material. Lack of a sharp diffraction pattern does not necessarily indicate the absence of that material.

The foregoing type of analysis that was

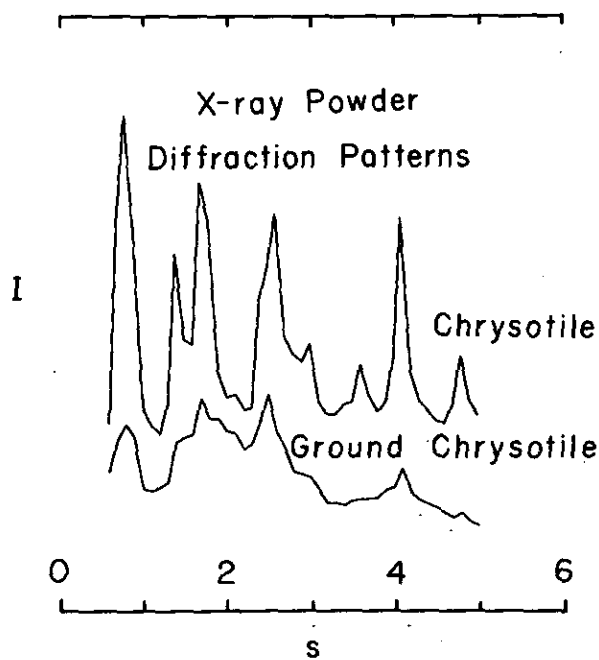


FIGURE 3. The x-ray powder diffraction patterns for chrysotile and chrysotile ground for 1 hr under toluene.

employed on the silica glass data can be used not only for amorphous materials but also for powdered crystalline samples. It may be used as a probe to analyze, on the atomic level, the effects on asbestos of grinding and chemical treatment which may alter the physical size of the particles, the local order, and even the basic atomic structure.

REFERENCES

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